

# Hamiltonian General Relativity and the Belinskii, Khalatnikov, Lifshitz Conjecture

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The Belinskii, Khalatnikov and Lifshitz conjecture says that as one approaches space-like singularities in general relativity, ‘time derivatives dominate over spatial derivatives’ so that the dynamics at any spatial point is well captured by an ordinary differential equation. By now considerable evidence has accumulated in favor of these ideas. Starting with a Hamiltonian framework, we provide a formulation of this conjecture in terms of variables that are tailored to non-perturbative quantization. Our formulation serves as a first step in the analysis of the fate of generic space-like singularities in loop quantum gravity.

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## I. INTRODUCTION

In 1970, Belinskii, Khalatnikov and Lifshitz (BKL) made a conjecture which, if true, would shed considerable light on the nature of space-like singularities in general relativity [1]. They suggested that as one approaches these singularities, time derivatives would dominate over spatial derivatives, implying that the asymptotic dynamics would be well described by an ordinary differential equation. At first this claim seems astonishingly strong. However, over the years considerable analytic and numerical evidence has accumulated in its favor (see, e.g., [2, 3, 4]). Together, these results suggest the following scenario: i) Geometry at any spatial point is well described by the Bianchi I metric for long stretches of time; ii) From time to time the parameters  $p_i$  characterizing the Bianchi I metric undergo a (Bianchi II) transition, rapidly settling to new values  $p'_i$ ; and, iii) The spatial gradients *can* grow but they do so on ‘small sets’ where spikes develop.<sup>1</sup> In addition, except for a scalar field or a stiff fluid, sources do not play much of a role in dynamics; ‘matter doesn’t matter’ close to the singularity.

It is tempting to use this scenario as a starting point in the analysis of what happens to these classical singularities in the quantum theory. In particular, Garfinkle [5] has suggested that understanding of the quantum behavior of the Bianchi I model would shed considerable

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<sup>1</sup> As is common in the recent literature, we use the convention that the singularity occurs at  $t = -\infty$ . So in general there are infinitely many transitions till one reaches the singularity. However, general relativity cannot be trusted once the curvature acquires Planck scale and until this epoch there are only a finite number of transitions and spikes at any spatial point.

light on the fate of space-like singularities in quantum gravity. It is now known in loop quantum cosmology that the Bianchi I singularity is naturally resolved because of quantum geometry effects [6, 7]. This suggests that there may well be a general result which says that *all* space-like singularities of the classical theory are naturally resolved in loop quantum gravity.

However, it is difficult to test this idea using the current formulations [8, 9] of the BKL conjecture. For, these formulations are motivated by the theory of partial differential equations rather than by Hamiltonian or quantum considerations. The basic variables, for example, are chosen to simplify functional analysis and numerics. While this is a natural strategy within classical general relativity, these variables are not well suited for quantum theory. For example, one often uses the variables  $\Sigma_{ab}, N_{ab}$ , introduced by Uggla, van Elst, Wainwright and Ellis (UEWE), which are obtained by dividing certain geometric fields by the trace  $K$  of the extrinsic curvature [8]. It is difficult to write down the corresponding operators in the quantum theory particularly because of the  $K^{-1}$  factors. So, the question arises: Is there a formulation of the BKL conjecture in terms of variables that are well suited for non-perturbative quantization? The answer turns out to be in the affirmative. The goal of this communication is to present a succinct summary of this formulation. As we will see, the framework has some features which make it appealing also in the classical theory.

We will focus on vacuum general relativity because ‘matter does not matter’. Details for the scalar field—which does matter—have been worked out and key differences will be summarized in section V.

## II. CONVENIENT VARIABLES

We will consider space-times  $(^4M, ^4g_{ab})$  with  $^4M = M \times \mathbb{R}$ , where  $M$  is a compact 3-manifold without boundary. Let us choose as our gravitational variables pairs  $(E_i^a, K_a^i)$  of fields on  $M$ , where  $a, b, c \dots$  are tensor indices and  $i, j, k \dots$  are  $\text{SO}(3)$  internal indices (which can be freely raised and lowered using the Cartan Killing metric on  $\text{so}(3)$ ).  $E_i^a$  represents an orthonormal triad on  $M$  (with density weight 1) and  $K_a^i$  represents extrinsic curvature ‘on shell’. These are canonically conjugate on the gravitational phase space [11, 12]:  $\{E_i^a(x), K_b^j(y)\} = \delta_b^a \delta_i^j \delta^3(x, y)$ .

The density weighted triad  $E_i^a$  determines a positive definite metric  $q_{ab}$  on  $M$  via  $E_i^a E_i^{bi} = q q^{ab}$  where  $q$  is the determinant of  $q_{ab}$ . The standard extrinsic curvature  $K_{ab}$  is given by  $E^{bi} K_{ab} = \sqrt{q} K_a^i$ . The scalar, vector and Gauss constraints of vacuum general relativity are given by

$$S := -q R - 2E_{[i}^a E_{j]}^b K_a^i K_b^j \approx 0, \quad V_a := 4 D_{[a} (K_{b]}^i E_I^b) \approx 0, \quad G^k := \epsilon_i{}^{jk} E_j^a K_a^i \approx 0, \quad (2.1)$$

where  $D$  and  $R$  denote the derivative operator and the Ricci scalar of  $q_{ab}$ . As usual, the Hamiltonian generating dynamics is just a linear combination of these constraints. The triad  $E_i^a$  determines a unique  $\text{SO}(3)$  connection  $\Gamma_a^i$  through  $D_a E_i^b + \epsilon_{ij}{}^k \Gamma_a^j E_k^b = 0$ . One can define another  $\text{SO}(3)$  connection  $A_a^i$  via  $A_a^i := \Gamma_a^i - \gamma K_a^i$  where  $\gamma$  is called Barbero-Immirzi parameter. Loop quantum gravity is based on the canonical pair  $(A_a^i, E_i^a)$ . This pair provides the point of departure for our formulation of the BKL conjecture.

In the classical analysis we now wish to undertake, it is simpler to use all three fields,  $\Gamma_a^i, K_a^i, E_i^a$ , although  $\Gamma_a^i$  is determined by  $E_i^a$ . The key idea can be then summarized as follows. The accumulated results to date suggest that the metric  $q_{ab}$  becomes degenerate

at the singularity, whence its determinant  $q$  vanishes there. (For example in the Bianchi I model, in terms of the commonly used proper time  $t$ , the metric is given by  $ds^2 = -dt^2 + \sum_i t^{2p_i} dx_i^2$  and the singularity occurs at  $t = 0$ . Since  $\sum p_i = 1$ , we have  $q = t^2$ .) Therefore one might expect that fields which are rescaled by appropriate powers of  $q$  would remain well behaved at the singularity. Similarly, while the covariant spatial derivatives  $D_a f$  of fields  $f$  may not be sub-dominant compared to time-derivatives, derivatives  $D_i f := E_i^a D_a f$  are more likely to be, because of the  $\sqrt{q}$  factor in the density weighted triad  $E_i^a$ . This strategy is similar to that used in a more common formulation of the conjecture [2, 4, 8] where, as mentioned in section I, one divides geometric fields by the trace  $K$  of the extrinsic curvature which is expected to diverge at the singularity. The relation between the two strategies is discussed in section III.

These motivations lead us to introduce the following basic variables:

$$C_i^j := E_i^a \Gamma_a^j - E_k^a \Gamma_a^k \delta_i^j, \quad \text{and} \quad P_i^j := E_i^a K_a^j - E_k^a K_a^k \delta_i^j. \quad (2.2)$$

It turns out that constraints can be re-expressed *entirely* in terms of  $C_{ij}, P_{ij}$  and their  $D_i$  derivatives:

$$S := 2\epsilon^{ijk} D_i(C_{jk}) + 4C_{[ij]} C^{[ij]} + C_{ij} C^{ji} - \frac{1}{2} C^2 + P_{ij} P^{ji} - \frac{1}{2} P^2 \approx 0 \quad (2.3)$$

$$V_i := -2D_j P_i^j - 2\epsilon_{jkl} P_i^j C^{kl} + \epsilon_{ijk} (2P^{jl} C_l^k - C P^{jk}) \approx 0 \quad (2.4)$$

$$G^k := \epsilon^{ijk} P_{ji} \approx 0. \quad (2.5)$$

Next, let us consider evolution equations, i.e., the Hamiltonian flow generated by the constraints. For simplicity, in this brief communication we will set the shift to zero. As in loop quantum gravity, our lapse  $N$  will be a scalar density of weight -1. Then the time evolution of our basic triplet  $(C_{ij}, P_{ij}, D_i)$  is governed by:

$$\dot{C}_{ij} = \frac{1}{2} \epsilon_j^{kl} D_k (N(2P_{li} - \delta_{li} P)) + N [2C_{(i|k|} P_{j)}^k + 2C_{[kj]} P_{i)}^k - P C_{ij}] \quad (2.6)$$

$$\dot{P}_{ij} = -\epsilon_j^{kl} D_k (N C_{li}) + \frac{1}{2} \epsilon_{ij}^k D_k (N C) - \epsilon^{klm} D_m (N C_{kl}) \delta_{ij} \quad (2.7)$$

$$\begin{aligned} & + 2\epsilon_{jk}^m C_{[ik]} D_m N + (D_i D_j - \delta_{ij} D^k D_k) N \\ & + N [-2C_{(ik)} C_{j)}^k + C C_{ij} - 2C^{[kl]} C_{[kl]} \delta_{ij}] \\ \dot{D}_i s_n &= \frac{n}{2} [D_i N P] s_n - N P_i^j D_j s_n \end{aligned} \quad (2.8)$$

where, in the last equation,  $s_n$  is any scalar density of weight  $n$ . These equations can be used as follows. On an initial slice, we construct  $(C_{ij}, P_{ij}, D_i)$  from a pair  $(E_i^a, K_a^i)$  of canonical variables. But then we can deal exclusively with the triplet  $(C_{ij}, P_{ij}, D_i)$ . The pair  $(E_i^a, K_a^i)$  satisfies constraints if and only if the triplet satisfies (2.3)–(2.5). Given such a triplet, we can evolve it using (2.6)–(2.8), *without having to refer back to the original canonical pair*  $(E_i^a, K_a^i)$ .

These two sets of equations have some interesting unforeseen features. First, the basic triplet  $(C_{ij}, P_{ij}, D_i)$  has *only internal indices*: our basic fields are *scalars* (with density weight 1). It would be of considerable interest to investigate if this fact provides new insights into the dynamics of 3+1 dimensional gravity [13]. Second, these equations do not refer to the triad  $E_i^a$ . Suppose we begin at an initial time where  $C_{ij}$  is derived from an  $E_i^a$ . Then these

constraint and evolution equations ensure that  $C_{ij}$  is derivable from a triad at all times. Furthermore, we can easily construct that triad directly from a solution  $(C_{ij}, P_{ij})$  to these equations: first solve (2.6)–(2.8) and then simply integrate the ordinary differential equation

$$\dot{E}_i^a = -NP_i^j E_j^a \quad (2.9)$$

at the end. Third, the structure of the constraint and evolution equations in terms of  $(C_{ij}, P_{ij}, D_i)$  is remarkably simple since only low order polynomials of these variables are involved. Finally, thanks to our rescaling by  $\sqrt{q}$ , our basic triplet  $C_{ij}, P_{ij}, D_i$  (as well as  $E_i^a$ ) is expected to have a well behaved limit at the singularity. (This expectation is borne out in the Bianchi I and II models.) Note also that our equations are meaningful even when the triad becomes degenerate. So, strictly (as in loop quantum gravity [11, 12]) we have a generalization of Einstein’s equations. To summarize, we have found variables which are likely to remain finite at the singularity and rewritten Einstein’s equations as a *closed system of differential equations* in terms of them. Therefore, this formulation may be particularly useful for proving global existence and uniqueness results.

However, in the formulation given above, all variables carry density weights. Also, although the operator  $D_i$  satisfies linearity and the Leibnitz rule, it is not a standard derivative operator: it has torsion and, more importantly, it changes the density weight by 1. These unconventional features may make these equations awkward to handle particularly for numerical work. In the detailed paper [10] we will provide an equivalent formulation involving only functions (with zero density weight) and a more familiar version of the operator  $D_i$ .

### III. THE CONJECTURE

The key step in any formulation of the BKL conjecture is to specify the basic variables, what one means by their ‘spatial derivatives’ (which are to be sub-dominant), and ‘time derivatives’ (which are to dominate). We will consider any smooth foliation  $M_t$  of an appropriate portion of  ${}^4M$  such that the space-like singularity of interest constitutes a (limiting) leaf. The time function  $t$  labeling our spatial slices is intertwined with the choice of lapse. We will assume that the density weighted lapse  $N$  admits a smooth limit as one approaches the singularity. Now, we are led by the intuition that the spatial metric  $q_{ab}(t)$  becomes degenerate at the singularity. This implies that the lapse function  $\bar{N}$  (with density weight zero), given by  $\bar{N} := \sqrt{q}N$ , goes to zero, i.e., that the singularity is at  $t = -\infty$ .

In this set up, our basic variables will be  $(C_{ij}, P_{ij})$  and the lapse  $N$ . By *time derivatives*, we will mean their Lie derivatives along the vector field  $t^a := \bar{N}n^a$  where  $n^a$  is the unit normal to the foliation  $M_t$ . By *spatial derivatives* we will mean their  $D_i$  derivatives. Since  $D_i := E_i^a D_a$ , the notion does not depend on coordinates. Rather, it is tied directly to the physical triads and the covariant derivatives compatible with the metric. Then, the idea behind the conjecture is that, as one approaches the singularity, the spatial derivatives  $D_i C_{jk}, D_i P_{jk}$  of the basic fields should become negligible compared to the basic fields themselves (in particular) because of the  $\sqrt{q}$  multiplier in the definition of  $E_i^a$ . An immediate consequence is that the antisymmetric part of  $C_{ij}$  is negligible [10], a fact that we will repeatedly use below.

Thus, our formulation of the BKL conjecture is that, as one approaches the singularity, solutions to the Einstein’s equations (2.3)–(2.8) are well approximated by solutions to the truncated system of equations obtained by ignoring the spatial derivatives. The truncated

constraints are purely algebraic equations:

$$S_{(T)} := C_{ij}C^{ji} - \frac{1}{2}C^2 + P_{ij}P^{ji} - \frac{1}{2}P^2 \approx 0 \quad (3.1)$$

$$V_i^{(T)} := \epsilon_{ijk}(2P^{jl}C_l^k - CP^{jk}) \approx 0 \quad (3.2)$$

$$G_{(T)}^k := \epsilon^{ijk}P_{ji} \approx 0, \quad (3.3)$$

while the truncated evolution equations are ordinary differential equations:

$$\dot{C}_{ij} = N[2C_{k(i}P_{j)}) - PC_{ij}] \quad \text{and} \quad \dot{P}_{ij} = N[-2C_{ik}C_{j}^k + CC_{ij}]. \quad (3.4)$$

Note that operation of truncation and hence the final truncated system depends crucially on one's choice of basic variables and notions of space and time derivatives. (For example, if we had used triads rather than  $C_{ij}$  as basic variables, we would have been led to set  $C_{ij}$  to zero in the truncation procedure, and truncation would have led us just to Bianchi I equations. The resulting BKL conjecture would have been manifestly false.)

How does this formulation compare with that of UEWE [4, 8]? In that framework, one divides the geometrical fields by the trace of the extrinsic curvature  $K$  (which is expected to diverge at the singularity) while here we multiply them by the volume element  $\sqrt{q}$  (which is expected to go to zero). There, the (scalar) lapse  $\bar{N}$  is such that  $\bar{N}K$  admits a limit  $\underline{N}$ . Therefore  $\bar{N}$  goes to zero and, as in our case, the singularity lies at  $t = -\infty$ . The key scale invariant variables  $(N_{ij}, \Sigma_{ij})$  which are expected to be well behaved at the singularity are related to our  $(C_{ij}, K_{ij})$  via

$$N_{ij} = 6P^{-1}C_{ij} \quad \text{and} \quad \Sigma_{ij} = -6P^{-1}P_{(ij)} + 2\delta_{ij}, \quad \text{or}, \quad (3.5)$$

$$C_{ij} = -\frac{K}{3}\sqrt{q}N_{ij} \quad \text{and} \quad P_{(ij)} = \frac{K\sqrt{q}}{3}(\Sigma_{ij} - 2\delta_{ij}). \quad (3.6)$$

Similarly the two sets of lapse fields are related simply by:  $N = \bar{N}K\sqrt{q}$ . Thus, although the motivations and the starting points of the two frameworks are quite different, the basic variables are closely related. From the viewpoint of differential equations, the two reduced systems would in essence be equivalent if  $K\sqrt{q}$  admits a finite, nowhere vanishing limit at the singularity. This condition holds for Bianchi I models (and also Bianchi II which describe the transitions between Bianchi I epochs). An advantage of the  $(C_{ij}, P_{ij})$  framework is that it is better adapted for non-perturbative quantization since it comes from the Hamiltonian framework underlying loop quantum gravity.

**Remarks:**

- i) In our formulation we have allowed a large class of foliations. However, a closer examination from the standpoint of differential equations may well lead to further restrictions. The inverse mean curvature foliations commonly used in conjunction with the UEWE framework appear to be well-suited also for our framework.
- ii) As a rule of thumb one often says that scale invariant scalars (such as  $N_{ij}$  and  $\Sigma_{ij}$ ) should have well-defined limits at the singularity. Those considerations can be extended to density weighted quantities used in this paper. The rule of thumb then is that a density of weight  $n$  has well-defined limit if it has scaling dimension  $2n$ . Since  $C_{ij}$  and  $P_{ij}$  have density weight 1 and scaling dimension 2, they should have a well defined limit at the singularity.
- iii) Consider the subspace of the full phase space on which  $D_i C_{jk} = 0$  and  $D_i P_{jk} = 0$  and demand that the lapse  $N$  satisfy  $D_i N = 0$ . Then, a non-trivial result is that the Hamiltonian

vector field of *full general relativity* is tangential to this sub-space; conditions  $D_i C_{jk} = 0$  and  $D_i P_{jk} = 0$  are preserved by the full evolution equations (2.6)–(2.8).

#### IV. THE BKL TRUNCATED HAMILTONIAN SYSTEM

Let us now explore the BKL truncated system we were led to in section III by focusing on the pair  $(C_{ij}, P_{ij})$ . We already know that  $C_{ij}$  is symmetric due to the BKL truncation. The Gauss constraint implies that  $P_{ij}$  is symmetric. Therefore, the basic variables of the truncated theory are pairs of *symmetric* fields  $(C_{ij}, P_{ij})$  on  $M$ .

Upon truncation, the full symplectic structure of general relativity yields the following Poisson brackets between these fields:

$$\begin{aligned} \{C_{ij}(x), C_{kl}(y)\}_T &= 0, \quad \text{and} \quad \{P_{ij}(x), P_{kl}(y)\}_T = 0, \\ \{P_{ij}(x), C_{kl}(y)\}_T &= (C_{k(j}\delta_{i)l} + C_{l(j}\delta_{i)k})(y) \delta^3(x, y). \end{aligned} \quad (4.1)$$

These are subject to the truncated scalar and vector constraints (3.1) and (3.2). This system of constraints is of first class. As before, for simplicity, let us set the shift to zero and obtain the evolution equations by taking Poisson brackets with the scalar constraint. The result is:

$$\dot{C}_{ij} = N [2C_{k(i}P_{j)}^k - PC_{ij}], \quad \text{and} \quad \dot{P}_{ij} = -N [2C_{ki}C_j^k - CC_{ij}]. \quad (4.2)$$

This is the Hamiltonian flow generated on the truncated phase space by the truncated constraints. It agrees with the evolution equations (3.4) of section III obtained by first using the full constraints on the full phase space and then truncating the full evolution equations. Thus, the truncation procedure is in complete harmony with the Hamiltonian framework.

To explore the structure of the truncated theory, it is convenient to solve and gauge fix the vector constraint. Since our fields  $C_{ij}$  and  $P_{ij}$  are now symmetric, the vector constraint (3.2) implies that, regarded as matrices, they commute, whence we can simultaneously diagonalize them. Finally, we can gauge-fix this constraint by demanding that  $C_{ij}$  and  $P_{ij}$  be diagonal. Then we arrive at the following description of the truncated phase space. It is coordinatized by the diagonal elements  $C_I, P_I$  of  $C_{ij}$  and  $P_{ij}$  (with  $(I = 1, 2, 3)$ ). Their Poisson brackets are given by:

$$\{C_I(x), C_J(y)\}_T = 0, \quad \{P_I(x), P_J(y)\}_T = 0, \quad \{C_I(x), P_I(y)\}_T = -2\delta_{IJ}C_J\delta(x, y). \quad (4.3)$$

There is a single (scalar) constraint:

$$S_{(T)}(x) := \frac{1}{2}(\sum_I C_I(x))^2 - \sum_I C_I^2(x) + \frac{1}{2}(\sum_I P_I(x))^2 - \sum_I P_I^2(x) \approx 0. \quad (4.4)$$

Thus, as expected, the truncated Hamiltonian system is ultra-local; dynamics at each spatial point is insensitive to what is happening elsewhere. Equations of motion are given by:

$$\dot{C}_I(x) = -NC_I(x) (\sum_J P_J(x) - 2P_I(x)), \quad \dot{P}_I(x) = NC_I(x) (\sum_J C_J(x) - 2C_I(x)). \quad (4.5)$$

Note that, although the constraint is symmetric under interchange of  $C_I$  and  $P_I$ , there is a basic asymmetry in the symplectic structure which descends to the equations of motion. Dynamics leaves the sector of the phase space with  $C_I \geq 0$  invariant. Let us focus on this

sector and set  $Q_I = -\ln C_I/2$ . Then,  $(Q_I, P_I)$  are canonically conjugate. Rewriting the constraint (4.4) in terms of  $Q_I$ , one immediately sees that what we have is particle dynamics in exponential potentials. By making a rigid rotation in the truncated phase space, (4.4) can be brought to the familiar Misner form [2]  $S_{(T)} = -\bar{P}_0^2 + \bar{P}_+^2 + \bar{P}_-^2 + e^{-(4/\sqrt{3})\bar{Q}_0} V(\bar{Q}_\pm)$ . However,  $\bar{Q}_0, \bar{Q}_\pm$  are components of a connection while the Misner variables refer to components of the 3-metric.

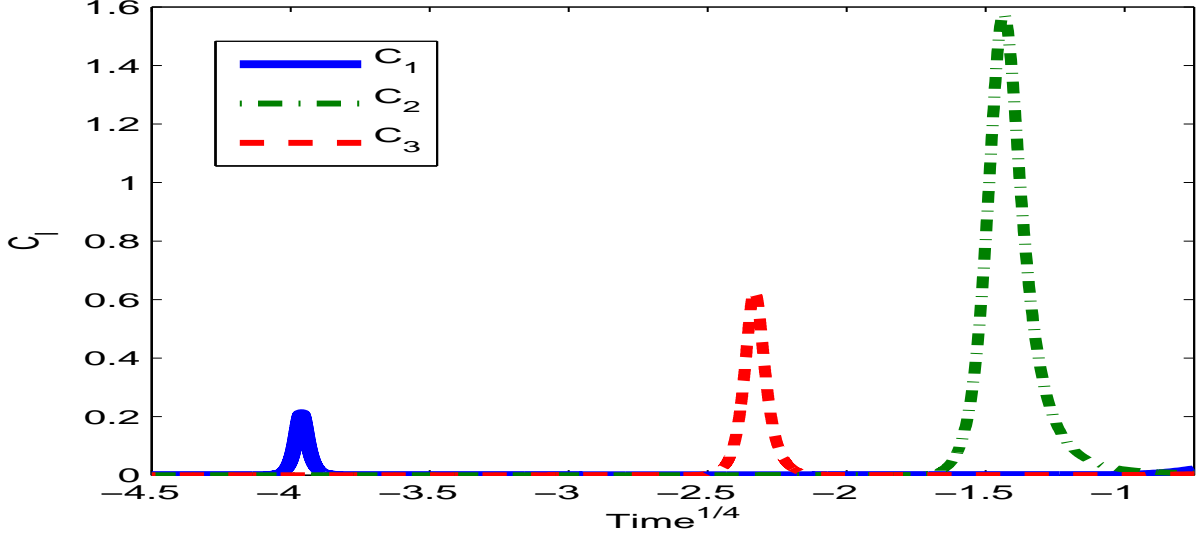


FIG. 1: Past evolution of the three  $C_I$  at a fixed point  $x$ , given by Eq (4.5). As time decreases,  $C_2$  starts growing rapidly near  $t = -1$ , reaches a peak, and then goes to zero rapidly. Then near  $t = -23$ ,  $C_3$  follows the same pattern and finally  $C_1$  does the same near  $t = -230$ . Their profiles are well described Eq (4.6). This growth and decay repeat ceaselessly as the singularity is approached at  $t = -\infty$ . In this simulation, the initial data at  $t = 0$  was  $P_1 = -0.4742, P_2 = -3.3586, P_3 = -1.3096; C_1 = 0.0746, C_2 = 0.0040, C_3 = 0.0070$ .

Note that if  $C_I(x)$  vanish initially at a point  $x$  in  $M$ , they remain zero throughout the evolution and  $P_I(x)$  remain constant. Then the dynamics of fields at that point  $x$  is that of the Bianchi I model.<sup>2</sup> (The  $P_I$  are linear combinations of the parameters  $p_i$  normally used to characterize the Bianchi I metric.) Dynamics of generic initial data is much more complicated than what one might expect from the deceptively simple form of the evolution equations (4.5). To get a handle on the Bianchi II transitions, one can linearize (4.5) about a Bianchi I solution. Since we have assumed that the universe contracts as  $t$  decreases, it follows that all three  $P_I$  of the Bianchi I solution are negative. One finds that as one evolves backward in time two of the three modes  $(C_I, P_I)$  are stable and one, with largest  $|P_I(x)|$ , is unstable. Let us suppose that  $|P_1(x)|$  is the largest. Then the exact evolution of the stable modes 2 and 3 is well tracked by the linearized equations which imply  $C_2(x, t) \approx 0 \approx C_3(x, t)$  and  $P_2(x, t) \approx P_2(x, t_0), P_3(x, t) \approx P_3(x, t_0)$ . However, for the unstable mode we have to use

<sup>2</sup> Note that since  $M$  is allowed to have any compact topology, it may not admit a global Bianchi I solution.

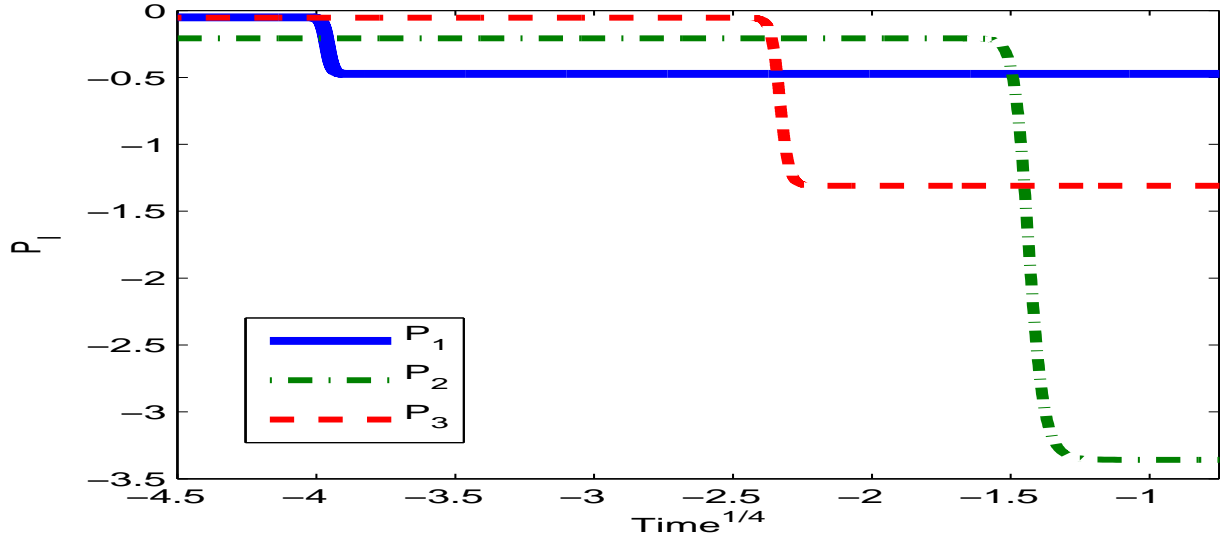


FIG. 2: Past evolution of the three  $P_I$  at a fixed point  $x$  (in the same simulation as in Figure 1). Their profiles are well described by Eq (4.7). Only one of the three  $P_I$  changes at a time, causing the solution to make a transition from one Bianchi I metric to another. The jump in each  $P_I$  is correlated in time with that in the corresponding  $C_I$ .

the full equations (4.5). Setting  $C_2 = C_3 = 0$  one obtains the solution:

$$C_1(x, t) = \pm 2(\sqrt{P_2 P_3} \operatorname{sech}(2\sqrt{P_2 P_3} N(t - \tau)), \text{ and} \quad (4.6)$$

$$P_1(x, t) = P_2 + P_3 + 2\sqrt{P_2 P_3} \tanh(2\sqrt{P_2 P_3} N(t - \tau)) \quad (4.7)$$

for some constant  $\tau$ , where the sign in the first equation is plus (minus) if  $C_1(x, t_0)$  is positive (negative). Thus, only one pair, namely  $(C_1(x, t), P_1(x, t))$ , evolves non-trivially. The form of solutions (4.6) implies that, as we evolve backward in time, there is a quick transition in which  $|C_1(x)|$  first increases, reaching a maximum value at  $t = \tau$ , and is then driven to zero, while  $P_1(x)$  is mapped to  $P_2(x, t_0) + P_3(x, t_0) + 2\sqrt{P_2(x, t_0)P_3(x, t_0)}$ . Simple algebra shows that this transition from one Bianchi I solution to another is given precisely by the well-known  $u$ -map. This derivation of the  $u$ -map does not require one to approximate the exponential potential in (4.4) by a rigid, perfectly reflecting wall. Also, our parametrization of the Bianchi-I solutions by  $P_I$  (rather than by the standard  $p_i$ ) makes it easier to follow the Bianchi II transitions both analytically and numerically because in any transition *only one* of the three  $P_I$  changes (while all three  $p_i$  change). Figures 1 and 2 show these transitions in a numerical solution to the ODEs (4.5). Here, an iterative Picard algorithm was used with an adaptive time step, chosen to ensure conservation of the scalar constraint. Such transitions in the truncated model mimic the situation in the full theory surprisingly well. (Compare, for example, our figures 1 and 2 with figures 5 and 4 in the second paper of [4]).

So far we focused on the dynamics at a single spatial point  $x$ . Let us now consider a 2-dimensional surface in the physical space on which one of the  $C_I$ , say  $C_1$ , vanishes and  $C_2, C_3$  are small. Fix a point  $x$  on this surface. Then,  $C_1$  is positive to one side of the



2-surface and negative to the other. At a point  $y$  in a neighborhood of  $x$ , as  $t$  decreases,  $C_1(y)$  first increases rapidly if it is initially positive and decreases rapidly if it is initially negative (following the  $\text{sech}(t - \tau)$  profile of (4.6)). This produces steep gradients at  $x$  for some time, which appear as spikes. However, as  $t$  decreases further,  $|C_1|$  goes to zero rapidly on both sides of the 2-surface for  $t < \tau$ . So the spike in  $C_1$  becomes dilute and disappears (but it will reoccur and disappear again repeatedly on further backward evolution).  $P_1$  on the other hand remains constant at  $x$  but decreases on either side of the 2-surface. As  $t$  decreases, the gradient of  $P_1$  keeps increasing and the spike sharpens. These transitions and spikes have been observed in numerous simulations of the truncated system [15]. However, because the spatial gradients become large at spikes, the truncated system becomes a poor approximation and one has to consider the full system (as, e.g., in [16]).

The analytical arguments given above explain all the qualitative features of the truncated dynamics if the initial phase space point lies in a neighborhood of a Bianchi I fixed point. But we do not have an analytical understanding of what happens away from this neighborhood. Numerical simulations show that even if one starts far away from pairs  $(C_I, P_I)$  corresponding to Bianchi I solutions, dynamics drives the system quickly to the Bianchi I sub-space. It would be very useful to have an analytical derivation of this phenomenon for our system (4.5) without having to make further approximations.

## V. DISCUSSION

We began with the Hamiltonian formulation of general relativity underlying loop quantum gravity where the basic fields are spatial triads  $E_i^a$  with density weight 1, spin connections  $\Gamma_a^i$  they determine, and extrinsic curvatures  $K_a^i$ . Based on the examples that have been studied analytically and numerically, the general expectation is that the determinant  $q$  of the spatial metric  $q_{ab}$  would become degenerate and the trace  $K$  of the extrinsic curvature would diverge at space-like singularities. One can therefore hope to obtain fields which remain well-defined at the singularity either by multiplying natural geometric fields by suitable powers of  $q$  or dividing them by suitable powers of  $K$ . In a commonly used UEWE framework [4, 8], one chooses to divide by  $K$ . The resulting fields satisfy differential equations with desirable properties. However, because of the presence of  $K^{-1}$ , in quantum theory it is difficult to introduce operators corresponding to the new fields.

We adopted the complementary strategy of multiplying geometrical fields by  $\sqrt{q}$ . In the Hamiltonian formulation with which we began, the basic field  $E_i^a$  is already obtained by multiplying the orthonormal triad by  $\sqrt{q}$ . One would therefore expect it to vanish at the singularity and this expectation is borne out in examples. Consequently,  $E_i^a$  also provides a natural avenue to construct additional fields needed in the BKL conjecture. Our variables  $C_i^j$  and  $P_i^j$  were obtained (modulo trace terms) simply by contracting the spatial indices of  $\Gamma_a^j$  and  $K_a^j$  by  $E_i^a$ . Furthermore, because  $E_i^a$  vanishes in the limit, the operator  $D_i := E_i^a D_a$  provides a convenient tool to express the notion of ‘*spatial derivatives which are to become subdominant*’ near the singularity. The main expectation is that asymptotically  $D_i C_{jk}$  and  $D_i P_{jk}$  would become ‘negligible’ relative to  $C_{jk}$  and  $P_{jk}$ . Now, in exact general relativity, time derivatives of  $C_{ij}$  and  $P_{ij}$  can be expressed in terms of their  $D_i$  derivatives, purely algebraic (and at most quadratic) combinations of  $C_{ij}$  and  $P_{ij}$ , the lapse  $N$  and its  $D_i$  derivatives (see (2.3)–(2.8)). Therefore, if in the limit the  $D_i$  derivatives of the basic fields become negligible compared to the fields themselves, we are naturally led to conclude that time derivatives would dominate the spatial derivatives. This chain of argument led to our

formulation of the BKL conjecture.

This rather simple idea depends on the fact that the structure of Einstein's equations has an interesting feature: as saw in section II, once the triplet  $C_{ij}, P_{ij}, D_i$  is constructed from the triad  $E_i^a$  and the extrinsic curvature  $K_a^i$  on an *initial slice*, the constraint and evolution equations can be expressed entirely in terms of the triplet. Given a solution to these equations, the spatial triad  $E_i^a$  (and hence the metric  $q_{ab}$ ) can be recovered at the end simply by solving a total differential equation, (2.9). This is a surprising and potentially deep property of Einstein's equation. It provided key motivation for our formulation of the BKL conjecture and could well capture the essential reason behind the BKL behavior observed in examples and numerical simulations. Therefore, an appropriate quantization of the truncated system, e.g., a la loop quantum cosmology, could go a long way toward understanding the fate of generic space-like singularities in quantum gravity.

Since the framework is developed systematically from a Hamiltonian theory, the BKL truncation naturally led to a truncated phase space. The specific truncation used has an important property: The truncated constraint and evolution equations on the truncated phase space coincide with the truncation of full equations on the full phase space. On the truncated phase space we could solve and gauge-fix the Gauss and vector constraints to obtain a simple Hamiltonian system. Solutions to this system have been explored both analytically [10] and numerically [15]. They exhibit the Bianchi I behavior, the Bianchi II transitions and spikes as in the analysis of symmetry reduced models [2] and numerical investigations of full general relativity [4].

Finally, in the main text we have restricted ourselves to vacuum equations. The addition of a massless scalar field is straightforward because the Hamiltonian framework with which we began can be easily extended to accommodate a scalar field [14]. The main features that are generally expected from the analysis of Andersson and Rendall [3] are reflected in the resulting truncated system. Thus, if the energy density in the scalar field is small, one again has Bianchi II transitions and spikes. However, once the energy density exceeds a critical value, these disappear and the asymptotic dynamics at any spatial point is described just by the Bianchi model with a scalar field without any transitions.

Derivations of analytical results and numerical simulations will appear in detailed papers [10, 15].

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